Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 01:35 PM BST

PDB ID	:	6QV4
Title	:	Crystal structure of the Ski2 RNA-helicase Brr2 from Chaetomium thermophilum bound to ATP-gamma-S
Authors	:	Absmeier, E.; Santos, K.F.; Wahl, M.C.
Deposited on	:	2019-03-01
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

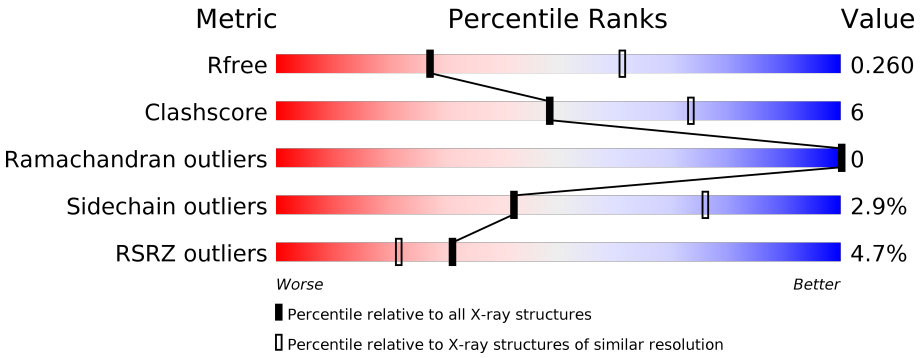
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1725	5% 79% 16%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13506 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Pre-mRNA splicing helicase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1666	Total	C	N	O	S	0	0	0
			13362	8544	2273	2481	64			

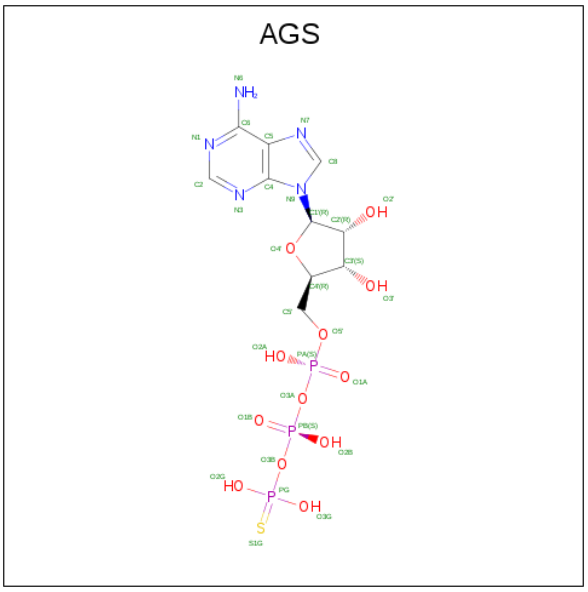
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	469	GLY	-	expression tag	UNP G0S0B9
A	470	ALA	-	expression tag	UNP G0S0B9
A	471	GLU	-	expression tag	UNP G0S0B9
A	472	PHE	-	expression tag	UNP G0S0B9

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

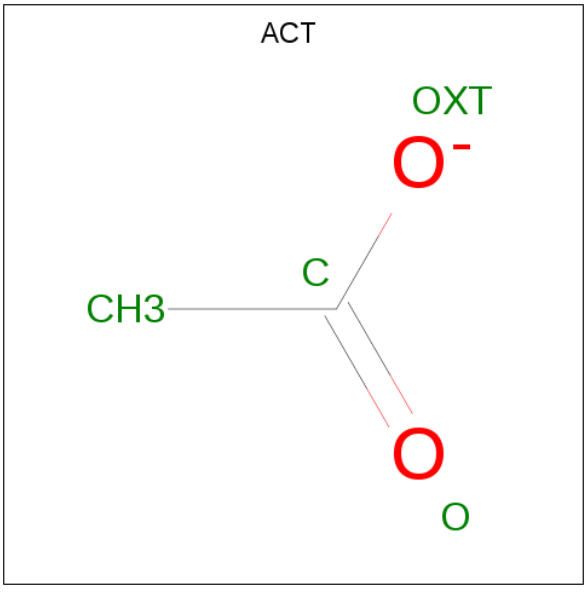
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Mn	0	0
			3	3		

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
3	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
3	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

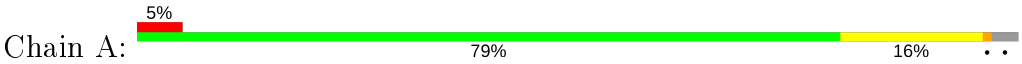
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	40	Total	O	0	0
			40	40		

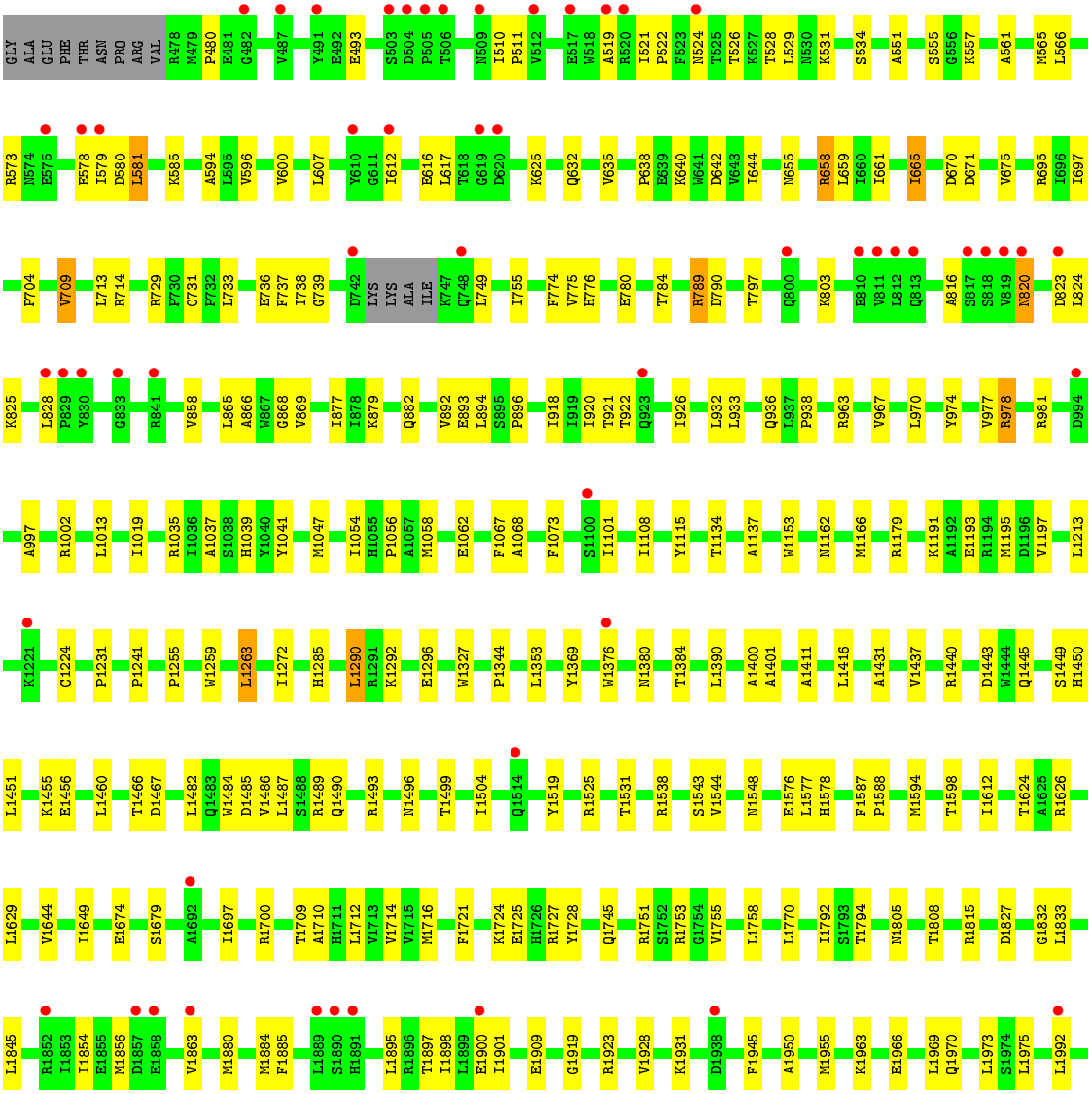
3 Residue-property plots (i)

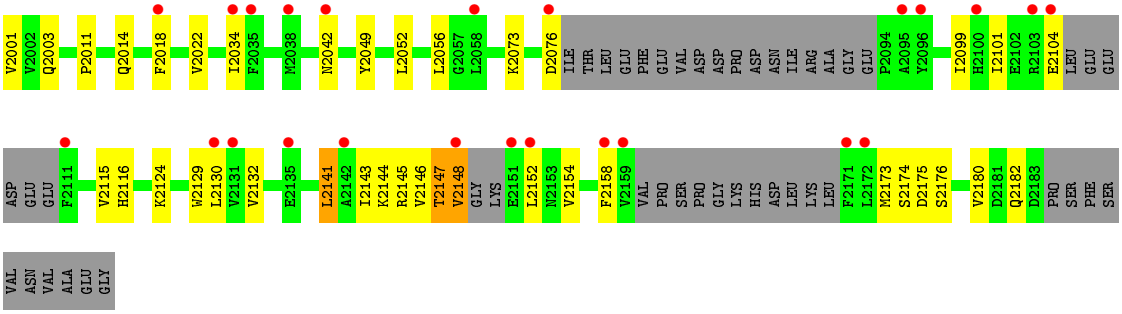
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Pre-mRNA splicing helicase-like protein

Chain A:






V2001 W2002 Q2003 P2011 Q2014 F2018 V2022 I2034 F2035 M2038 N2042 Y2049 L2052 L2056 G2057 L2058 K2073 D2076 ILE THR LEU GLU PHE GLU VAL ASP ASP PRO ASP ASN ILE ARG ALA GLY GLU P2094 A2095 Y2096 I2099 H2100 I2101 E2102 R2103 E2104 LEU GLU GLU
ASP GLU GLU F2111 V2115 H2116 K2124 W2129 L2130 V2131 V2132 E2135 L2141 A2142 I2143 K2144 R2145 V2146 T2147 V2148 GLY LYS E2151 L2152 N2153 V2154 F2158 V2159 VAL PRO SER PRO GLY LYS HIS ASP LEU LYS LEU F2171 L2172 M2173 S2174 D2175 S2176 V2180 D2181 Q2182 D2183 PRO SER PHE SER
VAL ASN VAL ALA GLU GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	124.82Å 124.82Å 127.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.53 – 2.80 44.53 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (44.53-2.80) 99.1 (44.53-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.209 , 0.260 0.209 , 0.260	Depositor DCC
R_{free} test set	3009 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	73.0	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 54.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.012 for -h,-k,l 0.033 for h,-h-k,-l 0.021 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13506	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, AGS, ACT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.24	0/13656	0.42	0/18520

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	13362	0	13423	161	0
2	A	3	0	0	0	0
3	A	93	0	36	1	0
4	A	8	0	6	0	0
5	A	40	0	0	0	0
All	All	13506	0	13465	162	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (162) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1255:PRO:HG3	1:A:1290:LEU:HD11	1.61	0.81
1:A:1460:LEU:HD22	1:A:1467:ASP:HB2	1.64	0.78
1:A:1431:ALA:HB3	1:A:1437:VAL:HG12	1.70	0.74
1:A:1485:ASP:OD1	1:A:1525:ARG:NH2	2.22	0.72
1:A:2130:LEU:HD11	1:A:2146:VAL:HB	1.74	0.69
1:A:1578:HIS:HB2	1:A:1755:VAL:HG12	1.73	0.69
1:A:1440:ARG:NH1	1:A:1443:ASP:OD2	2.29	0.65
1:A:816:ALA:O	1:A:820:ASN:ND2	2.29	0.65
1:A:1179:ARG:NH1	1:A:1193:GLU:OE1	2.30	0.64
1:A:1489:ARG:HB3	1:A:1794:THR:HG21	1.80	0.64
1:A:1037:ALA:HB2	1:A:1047:MET:HG3	1.81	0.63
1:A:581:LEU:HD13	1:A:632:GLN:HE21	1.64	0.62
1:A:784:THR:HG21	1:A:879:LYS:HE2	1.81	0.62
1:A:1709:THR:HG22	1:A:1745:GLN:HG3	1.83	0.61
1:A:2129:TRP:HB3	1:A:2143:ILE:HD11	1.82	0.60
1:A:2124:LYS:NZ	1:A:2175:ASP:OD2	2.29	0.59
1:A:573:ARG:HG2	1:A:579:ILE:H	1.67	0.59
1:A:2174:SER:H	1:A:2180:VAL:HG23	1.67	0.59
1:A:738:ILE:HD11	1:A:920:ILE:HG12	1.84	0.59
1:A:1068:ALA:O	1:A:1108:ILE:HD11	2.03	0.58
1:A:1197:VAL:HG11	1:A:1213:LEU:HD11	1.86	0.58
1:A:1058:MET:HG3	1:A:1062:GLU:HB2	1.84	0.58
1:A:1792:ILE:HG21	1:A:1854:ILE:HD11	1.85	0.56
1:A:776:HIS:CE1	1:A:894:LEU:HD21	2.41	0.55
1:A:511:PRO:HD3	1:A:534:SER:HB2	1.88	0.55
1:A:661:ILE:HD13	1:A:697:ILE:HB	1.88	0.55
1:A:617:LEU:HD21	1:A:644:ILE:HG13	1.88	0.55
1:A:825:LYS:HE2	1:A:828:LEU:HD11	1.90	0.54
1:A:1455:LYS:HG3	1:A:1456:GLU:H	1.73	0.54
1:A:1624:THR:HG22	1:A:1697:ILE:HD13	1.89	0.54
1:A:1259:TRP:HZ3	1:A:1290:LEU:HD23	1.72	0.53
1:A:729:ARG:HH22	1:A:733:LEU:HD13	1.73	0.53
1:A:970:LEU:HD23	1:A:1002:ARG:HG2	1.91	0.53
1:A:1450:HIS:O	1:A:1450:HIS:ND1	2.41	0.53
1:A:877:ILE:HG12	1:A:918:ILE:HB	1.91	0.53
1:A:1390:LEU:HA	1:A:1538:ARG:HH22	1.74	0.52
1:A:1966:GLU:O	1:A:1970:GLN:HG2	2.08	0.52
1:A:1445:GLN:O	1:A:1449:SER:OG	2.20	0.52
1:A:1598:THR:HG22	1:A:1714:VAL:HG11	1.90	0.52
1:A:1827:ASP:HB3	1:A:1832:GLY:HA3	1.90	0.52
1:A:1805:ASN:O	1:A:1808:THR:OG1	2.22	0.52
1:A:1577:LEU:HD11	1:A:1770:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1272:ILE:O	1:A:1285:HIS:HA	2.10	0.51
1:A:1380:ASN:O	1:A:1384:THR:HG23	2.11	0.51
1:A:521:ILE:O	1:A:524:ASN:ND2	2.44	0.51
1:A:2076:ASP:HB3	1:A:2104:GLU:HB3	1.92	0.50
1:A:1900:GLU:HG2	1:A:1945:PHE:CE1	2.47	0.50
1:A:1612:ILE:HG13	1:A:1710:ALA:HB2	1.93	0.50
1:A:561:ALA:O	1:A:565:MET:HG3	2.11	0.50
1:A:522:PRO:HG2	1:A:566:LEU:HD21	1.93	0.50
1:A:551:ALA:HB3	1:A:557:LYS:HD2	1.94	0.50
1:A:642:ASP:OD2	1:A:1041:TYR:OH	2.25	0.50
1:A:738:ILE:HD12	1:A:755:ILE:HG21	1.93	0.50
1:A:1231:PRO:HG2	1:A:1327:TRP:CD1	2.47	0.49
1:A:493:GLU:HG2	1:A:738:ILE:HG22	1.94	0.49
1:A:1056:PRO:HG3	1:A:1153:TRP:CE2	2.47	0.49
1:A:659:LEU:HD21	1:A:697:ILE:HG12	1.94	0.49
1:A:1724:LYS:HE2	1:A:1909:GLU:HB3	1.95	0.49
1:A:579:ILE:HG12	1:A:580:ASP:H	1.76	0.49
1:A:997:ALA:O	1:A:1002:ARG:NH2	2.46	0.48
1:A:573:ARG:HD3	1:A:578:GLU:HG3	1.96	0.48
1:A:585:LYS:HG2	1:A:632:GLN:HA	1.96	0.48
1:A:709:VAL:HG12	1:A:974:TYR:CE1	2.49	0.48
1:A:1115:TYR:CG	1:A:1134:THR:HG21	2.49	0.48
1:A:511:PRO:HD2	1:A:529:LEU:HB2	1.94	0.48
1:A:2147:THR:HB	1:A:2148:VAL:HG22	1.96	0.48
1:A:2144:LYS:HD2	1:A:2154:VAL:HG11	1.95	0.48
1:A:739:GLY:HA3	1:A:926:ILE:HD11	1.96	0.47
1:A:2115:VAL:HG11	1:A:2176:SER:HB2	1.96	0.47
1:A:736:GLU:HB3	1:A:918:ILE:HG13	1.95	0.47
1:A:659:LEU:HG	1:A:695:ARG:HB3	1.96	0.47
1:A:2042:ASN:HB2	1:A:2049:TYR:HB2	1.96	0.47
1:A:2129:TRP:HB2	1:A:2173:MET:HB2	1.96	0.47
1:A:1845:LEU:HD22	1:A:1863:VAL:HG11	1.96	0.47
1:A:1162:ASN:O	1:A:1166:MET:HG3	2.14	0.46
3:A:2205:AGS:O3G	3:A:2205:AGS:O2B	2.33	0.46
1:A:1598:THR:HG21	1:A:1716:MET:HE2	1.96	0.46
1:A:1496:ASN:HA	1:A:1499:THR:HG22	1.97	0.46
1:A:480:PRO:HG3	1:A:936:GLN:HG2	1.97	0.46
1:A:1067:PHE:HE1	1:A:1137:ALA:HA	1.81	0.46
1:A:1644:VAL:HB	1:A:1649:ILE:HD11	1.98	0.46
1:A:1895:LEU:O	1:A:1898:ILE:HG12	2.15	0.46
1:A:596:VAL:HG13	1:A:635:VAL:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:638:PRO:HB2	1:A:675:VAL:HG23	1.98	0.46
1:A:1969:LEU:HD22	1:A:2001:VAL:HG23	1.98	0.45
1:A:2052:LEU:O	1:A:2056:LEU:HG	2.16	0.45
1:A:510:ILE:HD11	1:A:531:LYS:HZ3	1.81	0.45
1:A:774:PHE:CZ	1:A:866:ALA:HB2	2.52	0.45
1:A:896:PRO:HA	1:A:932:LEU:HD11	1.98	0.45
1:A:1674:GLU:O	1:A:1963:LYS:NZ	2.48	0.45
1:A:2182:GLN:OE1	1:A:2182:GLN:N	2.50	0.45
1:A:921:THR:OG1	1:A:922:THR:N	2.49	0.45
1:A:978:ARG:HH21	1:A:981:ARG:HB2	1.82	0.45
1:A:1931:LYS:HE2	1:A:1931:LYS:HB3	1.81	0.45
1:A:1885:PHE:CE2	1:A:1975:LEU:HD12	2.52	0.45
1:A:1897:THR:O	1:A:1901:ILE:HG12	2.18	0.44
1:A:789:ARG:NH1	1:A:790:ASP:OD1	2.50	0.44
1:A:1400:ALA:HA	1:A:1543:SER:O	2.17	0.44
1:A:1626:ARG:HA	1:A:1626:ARG:HE	1.81	0.44
1:A:2011:PRO:HB2	1:A:2034:ILE:HG13	1.98	0.44
1:A:882:GLN:NE2	1:A:893:GLU:OE2	2.50	0.44
1:A:1576:GLU:HG3	1:A:1751:ARG:HD3	1.97	0.44
1:A:1712:LEU:HA	1:A:1753:ARG:O	2.17	0.44
1:A:581:LEU:HG	1:A:581:LEU:H	1.53	0.44
1:A:704:PRO:HG2	1:A:938:PRO:HA	1.98	0.44
1:A:1973:LEU:HD13	1:A:2124:LYS:HE3	1.99	0.44
1:A:519:ALA:HA	1:A:566:LEU:HD22	1.99	0.44
1:A:655:ASN:O	1:A:658:ARG:NH1	2.51	0.44
1:A:1390:LEU:HA	1:A:1538:ARG:NH2	2.32	0.44
1:A:1919:GLY:O	1:A:1923:ARG:N	2.38	0.44
1:A:729:ARG:HG3	1:A:731:CYS:H	1.82	0.44
1:A:823:ASP:OD1	1:A:824:LEU:N	2.48	0.44
1:A:1411:ALA:HB1	1:A:1504:ILE:HD13	2.00	0.44
1:A:977:VAL:O	1:A:981:ARG:HG2	2.17	0.44
1:A:526:THR:HG22	1:A:528:THR:H	1.83	0.43
1:A:1721:PHE:HB2	1:A:1728:TYR:CE1	2.53	0.43
1:A:519:ALA:HB1	1:A:566:LEU:HD13	2.01	0.43
1:A:1054:ILE:HG22	1:A:1153:TRP:HZ3	1.83	0.43
1:A:2003:GLN:HG3	1:A:2014:GLN:HE21	1.82	0.43
1:A:2022:VAL:HG13	1:A:2056:LEU:HD22	1.99	0.43
1:A:1369:TYR:CE2	1:A:1416:LEU:HB3	2.54	0.43
1:A:1401:ALA:O	1:A:1544:VAL:HA	2.19	0.43
1:A:1594:MET:O	1:A:1598:THR:HG23	2.18	0.43
1:A:1482:LEU:O	1:A:1486:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:LEU:HD13	1:A:612:ILE:HD11	2.00	0.42
1:A:775:VAL:HG11	1:A:780:GLU:HG3	2.01	0.42
1:A:1484:TRP:CE3	1:A:1487:LEU:HD11	2.54	0.42
1:A:892:VAL:HG12	1:A:893:GLU:H	1.84	0.42
1:A:737:PHE:CZ	1:A:933:LEU:HD12	2.55	0.42
1:A:1013:LEU:HB3	1:A:1019:ILE:HB	2.01	0.42
1:A:665:ILE:H	1:A:665:ILE:HG13	1.57	0.42
1:A:2099:ILE:HG12	1:A:2154:VAL:H	1.84	0.42
1:A:511:PRO:HD3	1:A:534:SER:CB	2.50	0.42
1:A:1490:GLN:HB3	1:A:1493:ARG:HG2	2.00	0.42
1:A:1950:ALA:HA	1:A:1955:MET:HE2	2.02	0.42
1:A:493:GLU:HA	1:A:738:ILE:HG22	2.01	0.42
1:A:1263:LEU:HD12	1:A:1327:TRP:HH2	1.85	0.41
1:A:1587:PHE:HB3	1:A:1588:PRO:HD3	2.02	0.41
1:A:967:VAL:HG22	1:A:1002:ARG:HB3	2.02	0.41
1:A:1241:PRO:HB2	1:A:1344:PRO:HD3	2.02	0.41
1:A:670:ASP:OD1	1:A:671:ASP:N	2.49	0.41
1:A:1292:LYS:O	1:A:1296:GLU:HG2	2.19	0.41
1:A:1449:SER:HA	1:A:1455:LYS:HB3	2.01	0.41
1:A:1449:SER:HB3	1:A:1455:LYS:HD3	2.02	0.41
1:A:2073:LYS:HG3	1:A:2116:HIS:HB2	2.03	0.41
1:A:600:VAL:HG21	1:A:616:GLU:HB2	2.02	0.41
1:A:1191:LYS:O	1:A:1195:MET:HG3	2.20	0.41
1:A:1548:ASN:HD22	1:A:1815:ARG:NH2	2.19	0.41
1:A:640:LYS:HD2	1:A:640:LYS:HA	1.88	0.41
1:A:1073:PHE:CD2	1:A:1108:ILE:HD12	2.55	0.41
1:A:1856:MET:HB2	1:A:1863:VAL:HG12	2.02	0.41
1:A:2130:LEU:CD1	1:A:2146:VAL:HB	2.47	0.41
1:A:1101:ILE:HD12	1:A:1101:ILE:H	1.86	0.41
1:A:594:ALA:HB1	1:A:868:GLY:HA3	2.02	0.41
1:A:775:VAL:HG12	1:A:776:HIS:H	1.86	0.41
1:A:1451:LEU:HD23	1:A:1451:LEU:HA	1.81	0.40
1:A:2141:LEU:HD21	1:A:2158:PHE:HD1	1.87	0.40
1:A:865:LEU:O	1:A:869:VAL:HG22	2.20	0.40
1:A:1598:THR:HG21	1:A:1716:MET:CE	2.51	0.40
1:A:1725:GLU:HB2	1:A:1727:ARG:HG2	2.04	0.40
1:A:1714:VAL:HG13	1:A:1755:VAL:HG23	2.02	0.40
1:A:625:LYS:HD2	1:A:644:ILE:HD11	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1654/1725 (96%)	1606 (97%)	48 (3%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1473/1523 (97%)	1431 (97%)	42 (3%)	42 76

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	555	SER
1	A	581	LEU
1	A	658	ARG
1	A	665	ILE
1	A	709	VAL
1	A	713	LEU
1	A	714	ARG
1	A	749	LEU
1	A	789	ARG
1	A	797	THR
1	A	803	LYS
1	A	820	ASN
1	A	858	VAL

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Mol	Chain	Res	Type
1	A	963	ARG
1	A	978	ARG
1	A	1035	ARG
1	A	1039	HIS
1	A	1224	CYS
1	A	1263	LEU
1	A	1290	LEU
1	A	1353	LEU
1	A	1376	TRP
1	A	1466	THR
1	A	1519	TYR
1	A	1531	THR
1	A	1629	LEU
1	A	1679	SER
1	A	1700	ARG
1	A	1758	LEU
1	A	1833	LEU
1	A	1880	MET
1	A	1884	MET
1	A	1928	VAL
1	A	1992	LEU
1	A	2018	PHE
1	A	2101	ILE
1	A	2132	VAL
1	A	2141	LEU
1	A	2145	ARG
1	A	2147	THR
1	A	2148	VAL
1	A	2152	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	AGS	A	2205	-	26,33,33	0.70	1 (3%)	26,52,52	0.96	2 (7%)
3	AGS	A	2206	2	26,33,33	0.73	1 (3%)	26,52,52	1.17	2 (7%)
4	ACT	A	2208	-	1,3,3	5.74	1 (100%)	0,3,3	0.00	-
4	ACT	A	2207	-	1,3,3	6.40	1 (100%)	0,3,3	0.00	-
3	AGS	A	2204	2	26,33,33	0.71	1 (3%)	26,52,52	1.02	2 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AGS	A	2205	-	-	5/17/38/38	0/3/3/3
3	AGS	A	2206	2	-	6/17/38/38	0/3/3/3
3	AGS	A	2204	2	-	2/17/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2207	ACT	CH3-C	6.40	1.56	1.48
4	A	2208	ACT	CH3-C	5.74	1.56	1.48
3	A	2204	AGS	PG-S1G	2.16	1.95	1.90
3	A	2206	AGS	PG-S1G	2.16	1.95	1.90
3	A	2205	AGS	PG-S1G	2.10	1.95	1.90

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2206	AGS	PA-O3A-PB	-4.49	117.43	132.83
3	A	2204	AGS	PA-O3A-PB	-3.35	121.32	132.83
3	A	2205	AGS	PA-O3A-PB	-3.00	122.54	132.83
3	A	2206	AGS	C5-C6-N6	2.26	123.79	120.35
3	A	2204	AGS	C5-C6-N6	2.26	123.78	120.35
3	A	2205	AGS	C5-C6-N6	2.25	123.77	120.35

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2206	AGS	C5'-O5'-PA-O1A
3	A	2206	AGS	C5'-O5'-PA-O2A
3	A	2206	AGS	C5'-O5'-PA-O3A
3	A	2206	AGS	O4'-C4'-C5'-O5'
3	A	2205	AGS	C5'-O5'-PA-O1A
3	A	2205	AGS	C5'-O5'-PA-O2A
3	A	2205	AGS	PB-O3A-PA-O5'
3	A	2204	AGS	C5'-O5'-PA-O3A
3	A	2205	AGS	PG-O3B-PB-O2B
3	A	2206	AGS	C3'-C4'-C5'-O5'
3	A	2204	AGS	PG-O3B-PB-O2B
3	A	2205	AGS	C5'-O5'-PA-O3A
3	A	2206	AGS	PB-O3A-PA-O2A

There are no ring outliers.

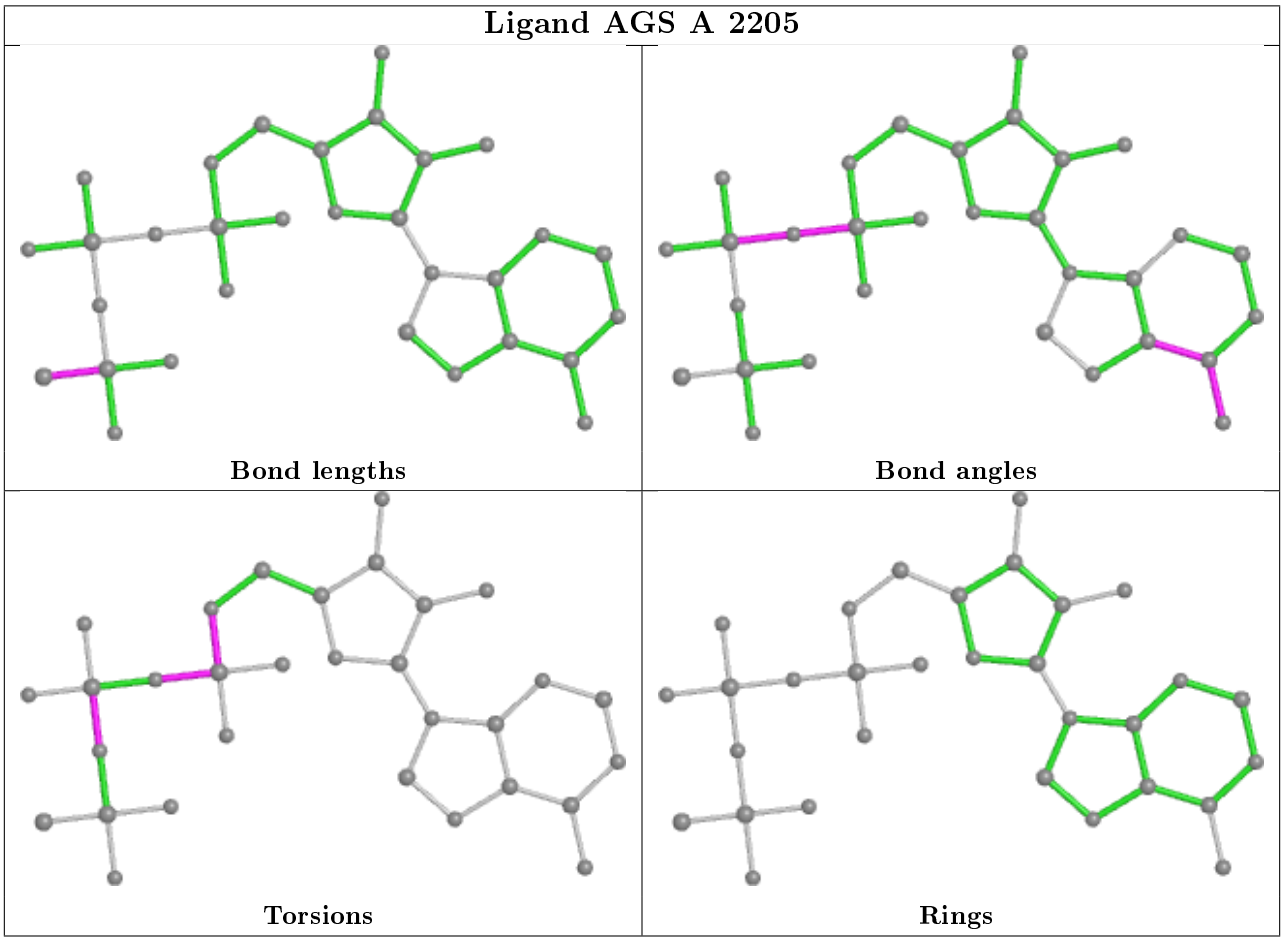
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2205	AGS	1	0

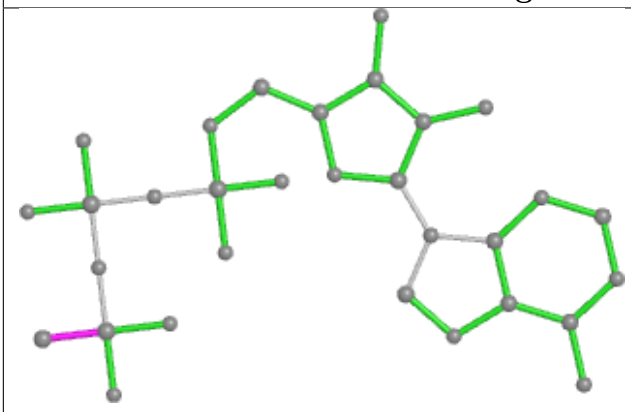
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

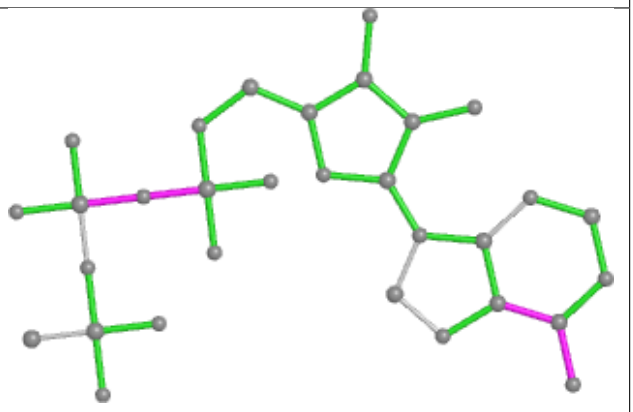
Ligand AGS A 2205



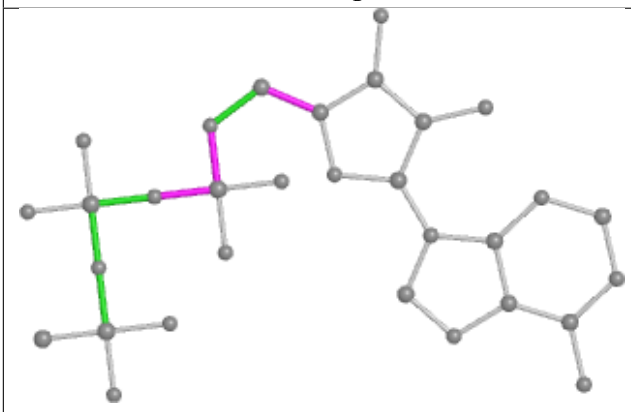
Ligand AGS A 2206



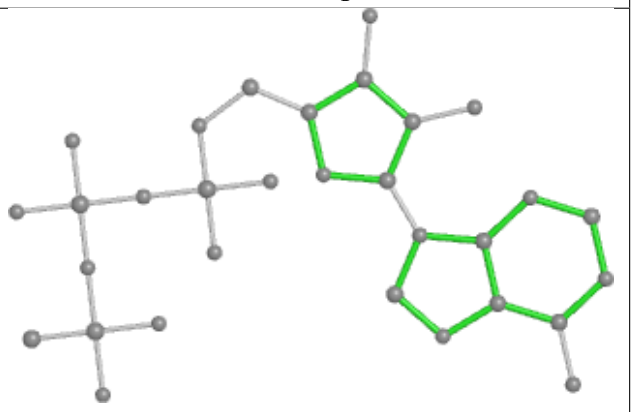
Bond lengths



Bond angles

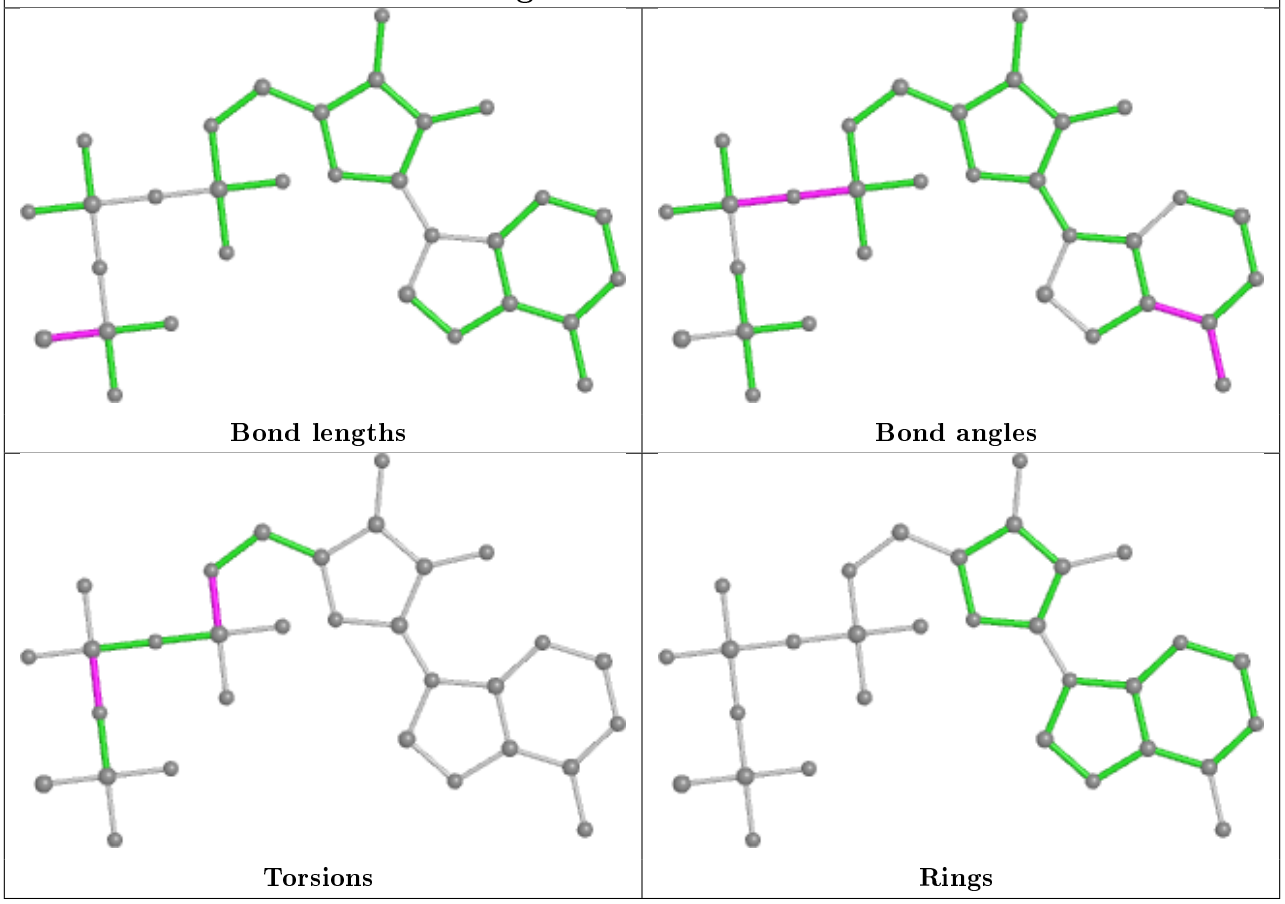


Torsions



Rings

Ligand AGS A 2204



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1666/1725 (96%)	0.16	78 (4%) 31 22	41, 84, 158, 219	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	748	GLN	6.7
1	A	2152	LEU	5.9
1	A	2142	ALA	4.8
1	A	578	GLU	4.8
1	A	2172	LEU	4.7
1	A	504	ASP	4.4
1	A	2076	ASP	4.3
1	A	2096	TYR	4.2
1	A	519	ALA	4.2
1	A	1890	SER	4.1
1	A	575	GLU	3.9
1	A	2158	PHE	3.9
1	A	1857	ASP	3.8
1	A	2151	GLU	3.8
1	A	819	VAL	3.6
1	A	1863	VAL	3.5
1	A	2135	GLU	3.5
1	A	2104	GLU	3.4
1	A	1891	HIS	3.4
1	A	610	TYR	3.4
1	A	579	ILE	3.4
1	A	994	ASP	3.3
1	A	820	ASN	3.2
1	A	1100	SER	3.2
1	A	620	ASP	3.1
1	A	2159	VAL	3.0
1	A	506	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	818	SER	2.9
1	A	1900	GLU	2.9
1	A	2095	ALA	2.9
1	A	810	GLU	2.9
1	A	2130	LEU	2.9
1	A	1858	GLU	2.8
1	A	828	LEU	2.8
1	A	2103	ARG	2.8
1	A	829	PRO	2.8
1	A	612	ILE	2.7
1	A	2111	PHE	2.7
1	A	1376	TRP	2.6
1	A	813	GLN	2.6
1	A	2042	ASN	2.6
1	A	619	GLY	2.6
1	A	509	ASN	2.6
1	A	2035	PHE	2.6
1	A	505	PRO	2.6
1	A	524	ASN	2.6
1	A	811	VAL	2.5
1	A	2058	LEU	2.5
1	A	2038	MET	2.5
1	A	520	ARG	2.5
1	A	833	GLY	2.5
1	A	1514	GLN	2.5
1	A	817	SER	2.4
1	A	812	LEU	2.4
1	A	2034	ILE	2.4
1	A	482	GLY	2.3
1	A	1938	ASP	2.3
1	A	923	GLN	2.3
1	A	800	GLN	2.3
1	A	1221	LYS	2.3
1	A	491	TYR	2.3
1	A	1692	ALA	2.3
1	A	517	GLU	2.2
1	A	2018	PHE	2.2
1	A	503	SER	2.2
1	A	2100	HIS	2.2
1	A	841	ARG	2.1
1	A	2131	VAL	2.1
1	A	1889	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	830	TYR	2.1
1	A	487	VAL	2.1
1	A	2148	VAL	2.1
1	A	823	ASP	2.1
1	A	512	VAL	2.1
1	A	742	ASP	2.1
1	A	2171	PHE	2.1
1	A	1852	ARG	2.0
1	A	1992	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

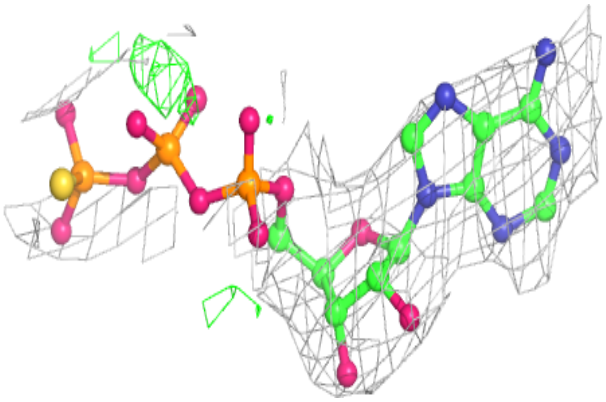
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

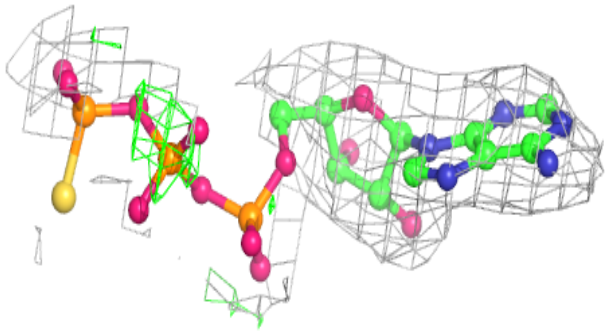
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ACT	A	2208	4/4	0.58	0.23	80,91,98,112	0
3	AGS	A	2204	31/31	0.87	0.20	114,125,153,161	0
4	ACT	A	2207	4/4	0.91	0.20	112,113,113,113	0
2	MN	A	2201	1/1	0.92	0.06	108,108,108,108	0
3	AGS	A	2206	31/31	0.92	0.19	51,69,107,124	0
2	MN	A	2203	1/1	0.93	0.17	106,106,106,106	0
3	AGS	A	2205	31/31	0.96	0.13	42,66,85,109	0
2	MN	A	2202	1/1	0.99	0.19	113,113,113,113	0

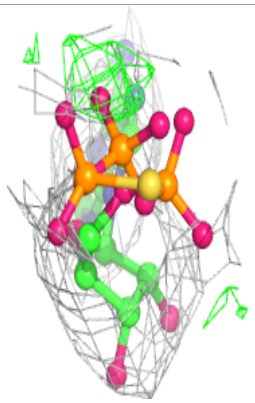
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around AGS A 2204:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

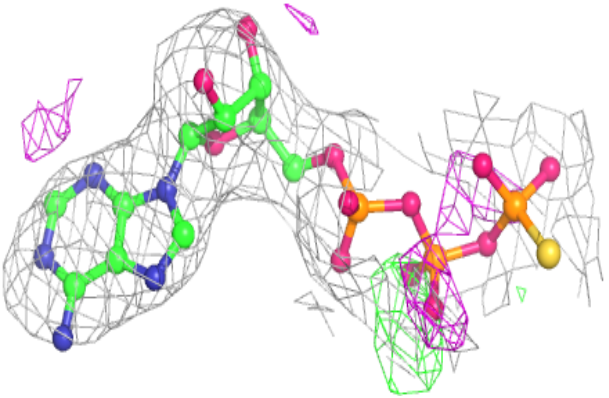


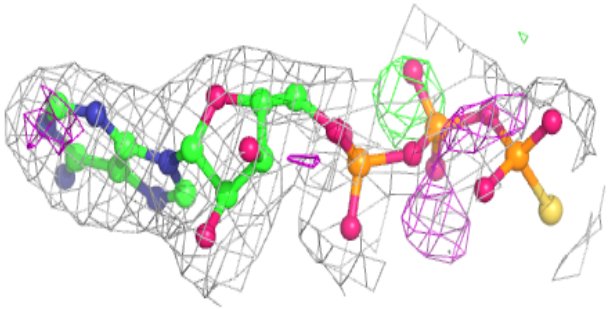


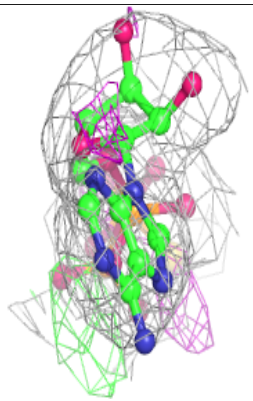


Electron density around AGS A 2206:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

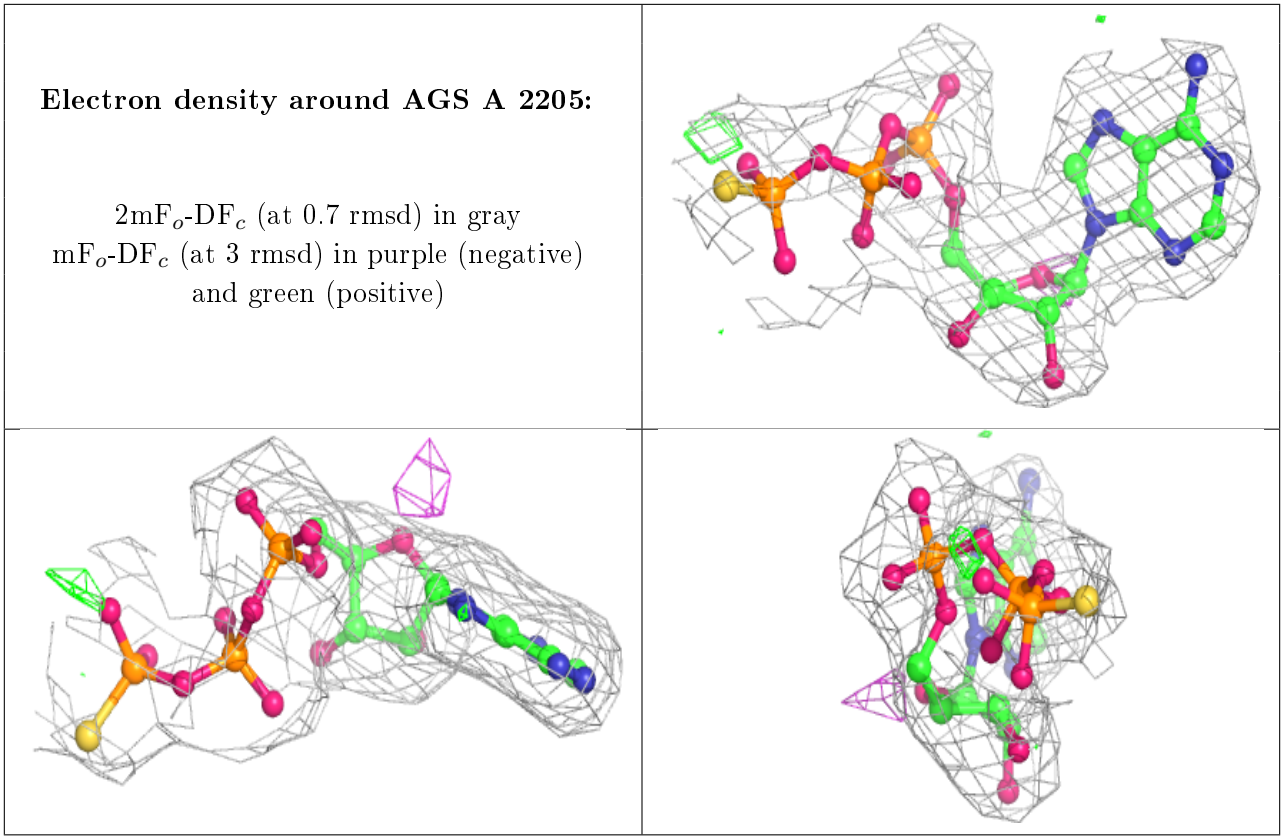






Electron density around AGS A 2205:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.